# Advanced Materials Experimentation and Analysis System

## 1. Background and rationale

The DOE weapons complex has always demanded the use of the most advanced manufacturing and materials analysis techniques. These techniques now require the ability to rapidly integrate diverse sets of experimental data over the lifetime of a operational system. This can include digital microscopy, electron microscopy, computed tomography, metallographic spectral data, eddy current and thermal data, to name a few. Even this data would only form part of the complete documentation of the design, fabrication and performance of a complex mechanical system. Integrating such information for easy interpretation by a team of engineers by providing advanced analytical and navigational capabilities would mark the establishment of a crucial new capability for the Advanced Design and Production Technology (ADaPT) program being undertaken at the DP Laboratories. In addition, this would be a new capability for the U.S. manufacturing industry - a capability that meets an increasingly important need as more advanced digital data acquisition tools become commonplace.

The typical method of dealing with such complex data is to build a log of experimental parameters, observations and analyses of the particular data and send copies to the collaborator, such as an another experimenter or a theoretician who wishes to apply theoretical design or simulation models to the data. Discussions are typically in person or over the telephone. There are numerous difficulties with this approach. First, it is hard to keep the various data linked together so that the experiment can be repeated or extended. The large volumes of images or related data make keeping them in a typical online system difficult. It may be difficult to go back and find related experimental data in the future. In addition, if this is done only on a local computer, it may be difficult to obtain, on demand, the compute power required for the analysis.

To resolve this problem we propose a radical departure in procedure which will change the way digital microscopy and imaging, as well as material science research and engineering, is performed. We propose to develop an integrated system for the acquisition, analysis, distribution, and collaborative exploration of digital microscopy and related multidimensional image data including metallographic spectroscopy. The system would be based on the distributed object technology developed in the Sunrise project, which has already been successfully applied in the multimedia computerized patient record system known as TeleMed. The new system would provide for simultaneous access and analysis of digital experimental data between two or more researchers at remote locations, as well as the ability to do selective analysis and correlation of results. It will enable the integration of chemical, spectral, and image data in a dynamic manner, as well as provide the security to control access to sensitive information.

## 2. Program development opportunity/new revenue

The systems approach we are proposing is completely consistent with and supportive of the ADaPT program by providing mechanisms for accelerating the development and deployment of materials and manufacturing technologies. In discussions we have already had with industry, we have found that not only is there not a product which provides the support we propose, but there is a great need for such a system in a variety of manufacturing industries. It will provide the seeds for a new way of managing the nuclear weapons stockpile as well as providing the knowledge base required for advanced development. After developing a prototype, we will engage industrial partners who would make some of this technology commercially available as it matures in much the same manner as we have been able to accomplish in the Sunrise project. We believe we can provide a strong integration between the ADaPT and ASCI programs by utilizing common tools across the entire design, development, and verification phases. The particular projects which we propose to support through our team approach are of fundamental importance to developing facilities for stockpile repair and rebuild characterization and realization. With this effort as a foundation, we see this technology spreading to many more weapons application areas as the program evolves and grows. This capability will also open up the possibilities of utilizing high performance computing in a variety of new ways of importance to the weapons engineering enterprise.

By substantially advancing the state of the art in this area to enable more rapid analysis and understanding of materials used in manufacturing, the laboratory will be a leader and substantially change the way industry deals with manufacturing technology. We anticipate a number of CRADA's with some of the manufacturers of digital microscopy equipment as well as with software firms which are providing analysis tools.

## 3. Connection to strategic directions and laboratory goals

In the area of Tactical Goals, this project will strongly support the following:

Science-based Stockpile Stewardship
Modeling, Simulation, and High Performance Computing.
The Plutonium Legacy
Develop industrial partnerships

Within the technical competencies, this project will provide support for a variety of areas in very novel ways be creating relationships that have not existed before.

Advanced materials Synthesis, Characterization and Processing
Advanced Computing, Modeling, and Simulation
Advanced Manufacturing Process and Technology
Nuclear Science and Technology

## 4. R&D approach and likelihood of success

The approach we are taking will involve the use of two closely related state-of-the-art weapons materials research efforts combined with state-of-the-art computational tools to enable efficient storage, retrieval, and analysis of experimental data in a way never done before in this field. This integrated approach has proven to be exceptionally powerful paradigm in the highly successful Sunrise project. We utilize significant applications to drive advanced computational environments in ways that are of primary value to the end user. To describe this approach, we break this discussion up into the various components under consideration: ***Applications, Concept Extraction, Distributed Data Storage, and Multimedia Collaborative Tools***

### *Applications*

#### *Analysis of Be-Al welds*

Current welding techniques for beryllium use aluminum as a filler metal and result in weld metal compositions which include varying amounts of Al with various microstructures. The morphology and grain size in the weld depends on many things, including the solidification rate.

For example, joining processes can produce a weld metal which in some cases is mainly Al, but may contain anywhere between 10 and 50% Be. Various defect structures, microstructures and grain sizes have been observed in Be welds, depending on the joining process. Mechanical properties of welds which contain a mixture of Be and Al, and especially properties of these welds at elevated temperatures, are not fully understood. It is proposed to use advanced quantitative techniques to study the distribution of Be in Al for various welds, and then relate this to the mechanical properties of the welds. The distribution of Be in Al is dependent on factors such as the gradient in solidification rate along the weld cross-section. Using techniques such as x-ray tomography, a full three-dimensional model of a weld can be examined. With this model, and the aid of advanced 3D image analysis, a quantitative representation of the weld can be developed. Along with mechanical properties of welds with varying microstructures, this quantitative representation can be used to develop a predictive model which relates the weld microstructure to its mechanical properties. It is expected that a predictive model can be developed for welding Be with Al. This has the advantage that, in lieu of an extensive (and expensive) experimental program, it would be possible to predict the properties of welds in Be based on their microstructures, and eventually relate these back to the weld parameters.

Preliminary data produced by LLNL used the synchrotron at Stanford to image electron beam welds of Be using an Al filler. These welds were produced at Los Alamos as part of parametric welding studies in support of the Pit Rebuild program. This technique has demonstrated the resolution necessary to image the characterize microstructural features of interest. The ability to analyze these large complex data sets provide an added dimension to understanding the spatial relationships of structures within the weld region. Quantitative analysis of data sets such as these, combined with BeAl mechanical properties data, will provide critical insight into the properties of welds representative of existing welds within the stockpile such as those produced by the PIGMA (Pressurized Inert Gas Metal Arc) process. The goal would be to enhance our knowledge and predictive capabilities related to the effect of component aging on the weld. The analysis of weld samples produced by new candidate joining processes such as laser an electron beam welding and using new BeAl alloys, will be enhanced by development of this capability. Funding has already been identified to support development of these new welding techniques under programs such as ADaPT.

This proposed effort would require a collaborative effort between Los Alamos ( ACL, MST, others) and LLNL to identify funding, benefits to weapons programs and dual use drivers. Benefits to the development of this technology could extend beyond DOE weapons programs to the private sector, specifically the characterization of laser welding techniques as applied to the joining of light weight alloys.

### *Aging of weapons materials*

As long-term storage of nuclear assets is currently a reality, it will be necessary to further our knowledge of potential changes to these materials. Understanding the mechanism and formation of helium bubbles in aged plutonium samples will be essential to the welfare of our nuclear stockpile. A suite of technologies to further investigate the microstructures, defect structures, and radiation damage effects of phases of aged plutonium are being proposed. These include direction observations of defects such as dislocation structures, precipitates and voids through the digital image analysis of TEM (Transmission Electron Microscope) images. This would be done in aged material from site returned warheads as well as other materials . Analysis tools will also include a laser-induced plasma spallation technique to determine spall strength based on He content and thermal history. The ability to rapidly compare the variety of data associated with a sample or series of samples and determine relationships between the thermal history, and the micrographic structure observed in the TEM will speed the progress of the research and the ultimate benefit to the weapons program.

## Concept Extraction:

Huge volumes of image data can be generated through the use of imaging techniques such as TEM and synchrotron x-ray microtomography. It is not only important to provide transparent distributed access to this data, but it is also important to provide intuitive software tools for data analysis. Users of the proposed system are not interested in data visualization (such as volume rendering techniques) as the ultimate goal of their research. Instead, they want to see visualizations and also obtain answers to specific questions about the imagery, such as, “In what areas of this sample do helium bubbles seem to develop most readily?”. Or they might want to obtain a quantitative analysis of the defects in a small weld (i.e. “What percentage of the material in this weld suffers from significant areas of defective Be-Al bonding?”).

“Concept Extraction” is a technique that has been previously explored as a data mining tool that promotes a strong collaboration between human users and computer analysis packages. The premise behind this technique is that computers are good at working on certain kinds of data processing problems (such as finding correlations in huge amounts of data), whereas humans are better at other tasks (such as interpreting what the correlations mean with respect to the problem at hand). We propose to develop concept extraction tools as part of this project that will enable materials researchers to interact easily with the tremendous volumes of 2-D and 3-D data that will be collected. Data mining tools will automatically find similar-looking regions within each 2-D or 3-D data set, and the user will categorize these regions by their “meaning” (i.e. pure Al, pure Be, strong Be-Al bond, weak Be-Al bond, defect, etc.) This categorization will be performed through the use of an interactive data analysis tool that allows the user to efficiently and effectively categorize this data. Because all correlations amongst the data will be identified off-line by the computer, the user will need to invest very little time in this part of the analysis process. The user can then generate a quantitative analysis report, or ask other specific questions about the data. The exact nature of these questions will be determined by the materials researchers themselves. This methodology has already been successfully applied to LANDSAT and medical x-ray data.

## Distributed Data Repositories:

A key piece of the materials properties data repository system is to provide coherent, yet distributed, access to the data. Access must take on several forms. One must be able to deposit various types of data into the system, retrieve that data for viewing or analysis, and be able to deposit the results of that analysis back into the data repository. When a scientist deposits data into the system the data must be organized so it is readily accessible. It must be possible to search the data for various materials properties, process input parameters, analysis results, or other features of the data.

The various instruments which provide data on materials of interest are located throughout the laboratory and the country. Therefore it must be possible to deposit data directly in the distributed repository from anywhere on the Internet. Furthermore, researchers and collaborators are located throughout the laboratory and the country. They also must be able to access their data from anywhere on the Internet. In the proposed system, researchers at Stanford University’s synchrotron will image electron beam welds and insert the data directly into the data repository system. Immediately, authorized researchers at Los Alamos and elsewhere will be able to examine the data to make certain features they are interested in have been captured and analysis can start. Such a system will enable a new generation of “on-line facilities”. Beyond the immediacy of access mentioned here, the data will be always be accessible using consistent mechanisms. As new analysis tools are developed they can be placed on the appropriate machine in the network and have full access to the repository and to other tools in the environment.

One of the key issues for the data repository is to be able to handle temporal data to study issues such as aging of materials and welds, or to do before/after studies on materials being subjected to mechanical or thermal stress. The Sunrise/TeleMed system was designed for easy access to just such temporal data. Although in the context of TeleMed we show the medical reports and images depicting a patient’s health and various physician “interventions” (drug prescriptions, etc.) over time, the principle is the same.

The Sunrise system stands as an elegant framework in which to place the materials repository. Many of the features required in a materials properties visual data repository system are Sunrise core technologies and embodied in the Sunrise/TeleMed system. New facilities needed, such as the ability to handle new data types and analysis operations specific to the materials community, are orthogonal and complimentary to features already in the system and can be added gracefully.

Sunrise is built on the industry standard distributed object technology known as the Common Object Request Broker Architecture or CORBA. CORBA objects refer to the computer science notion of objects which encapsulate data and functionality to manipulate that data in a single package. Objects allow more flexible system designs which can more readily adapt to new requirements. Objects allow standard manipulators of the data to be written once and used repeatedly.

Sunrise distributed objects are stored in a commercial object-oriented database system. An object-oriented database system allows for rapid development of the system, because developers do not need to spend time working around the critical deficiencies of relational database systems: the inability to manage arbitrary data types, the inability to naturally model hierarchical data structures, and the inability to deal with aggregate data structures. All of these three features are important in efficiently implementing and managing the materials properties data respository system. Furthermore, with an object-oriented database system, application developers can take full advantage of methods to encapsulate arbitrary programs with stored data, and multiple inheritance to reuse existing database schema design and methods.

Distributed objects, that is objects and references to objects distributed between programs on multiple computers, have several desirable features. They enable standard manipulations or computations to be performed on the data at the data repository or wherever in the network it is appropriate. This is preferable to the scientist moving the data to his/her workstation or to some other machine such as a supercomputer to perform the calculation. Distributed objects allow scientific workstations or PCs alike to control CPU intensive computations being performed on appropriate high performance machines regardless of data location throughout the network. It is possible to define complex objects that are comprised of other objects but independent of their actual locations. Clients can use the complex object and access its components as if the components were at the same source.

Distributed objects allow a convenient structure for packaging and organizing data and the codes which are needed to access that data at some time in the future. Coarse-grain objects are used to organize data on a particular material sample by containing finer-grain objects holding images or other spectral data from various instruments (TEM, XTM, etc.), analysis results, and commentary on sample significance. This method can improve the understandability and manageability of a scientist’s research legacy by matching the storage methods to the scientific content.

Much of the materials data is sensitive or corporate proprietary data. Authentication and authorization controls on the raw data and the analytical data is required. Because of the sensitive nature of medical records, Sunrise has developed a security infrastructure comprised of interfaces which allow the data to be held private according to entries in an authorization database. In the Sunrise system, users and software systems must be "authenticated" to use the system; that is their identity must be proven to other pieces of the system. Once authenticated, that user is authorized to see only specific information according to the authorization database. Once a user is authorized to see specific data, certain portions of that data may be encrypted while it is transmitted to the user. This is to prevent unauthorized eavesdropping of network traffic which is a major concern on wide area networks today. Our system is much more flexible than most in that specific portions of the data may be encrypted or not according to the sensitivity of the data and thus the definition of the object.

## *Collaborative Multimedia User Interface*

The user interface for this system will employ the same visual metaphor strategy that has already been applied so successfully to the TeleMed multimedia computerized patient record system. This metaphor represents the contents of a user's database by a collection of icons, each of which upon activation, takes the user directly to information of interest. This approach will permit easy access to digital experimental data and provide the ability to do selective analysis and correlation of results. Moreover, it will enable seamless integration of chemical, spectral, and image data.

As examples, consider the requirements of working with digital microscopy data and with X-ray tomographic investigations of metallic welds. In the former case, microscopy samples of varying magnifications can be easily accessed by positioning a slider which represents the range of magnifications available. The requested image will appear in a separate window. Then, clicking on a selected part of the image will cause ancillary spectral data to appear for the designated area. It will also be possible to create montages of selected images, data, and text, the aggregate of which can be saved as additional information in the database. For studies of X-ray tomography of welds, the user will be able to manipulate selected image slices as in the microscopy example, but there will be a 3D data manipulation capability, as well. Thus, the constituent slices in a tomographic dataset can be viewed as a dynamically constructed and rendered 3D volume. There will be tools for arbitrary orientation of the volume in 3-space and for highlighting selected features by contrast control.

Users of the system, regardless of domain, will be able to append a wide range of annotations to selected data items or aggregates of items. These annotations include textual "Post-it" notes, voice or other sound data, stored video fragments, and a general mark-up and sketching capability. Moreover, an audit trail facility will be an integral part of the system, providing information on who made what changes to the database and when they were made. These capabilities are already part of the TeleMed system.

A new and powerful feature of the user interface will be embedded collaboration. Colleagues-at-a-distance will be able to simultaneously interact with a database and discuss and analyze significant features together. As a minimum, collaborators will have the option of desktop videoconferencing, where they may see and talk to each other as they conduct their work. Most important, however, the system will provide a general shared whiteboard facility. This means, for example, that when one participant marks up a microscopy image, all other collaborators will see that action in real time. The final results of such a collaboration can be saved in the (common) database, whether it is a history of whiteboard sharing, the videoteleconference, or both.

## 5. Schedules and major milestones; expected scientific/technical results

At the end of the 1 year project, we will deliver a functional data handling tool which will be able to store and retrieve data and enable distributed collaborative data analysis. During the first month of the project will develop a set of requirements for the major application areas which will include the determination of the various concepts which will be used in the data analysis. These may include definition of useful analysis tools such as histograms, volume analysis, artifact removal, noise reduction, morphological feature definitions, and statistical properties to be used in cluster analysis. The next two months will be used to design the basic object structures required for data representation by the applications (building on sets of generic objects we will have already developed). At the same time the integration of video collaboration capabilities will be developed. The second quarter will be used to implement the object design. The integration of the data into the application framework and the validation of the system for use by the materials researchers will be accomplished during the second half of the year. This will build on the experience obtained from some very early prototypes which will be evaluated by the materials researchers. These early prototypes will be used by the materials researchers to evaluate to usefulness of the analysis tools on real Be weld data as well as helium bubble data from various sources. Approximately midway through the year we will engage various manufacturing companies and their software suppliers as to the possibility of bringing this software into the commercial market.

## 6. Related laboratory capabilities and investigator’s expertise

This project involves core parts of the laboratory involved with the weapons fabrication and evaluation of existing weapons components. The experimental facilities used in the data acquisition are state of the art. MST-5 already deals with a wide range of “customers” for the acquisition and analysis of experimental materials image data. These range from High Temperature Superconductivity experiments to structural materials for a variety of manufacturing processes, both within the laboratory and in commercial industry. In addition, this project involves a team which already has successfully demonstrated the data management technology described here in another application called TeleMed which has proven to be a leading technology of enormous interest in the healthcare industry. For example, it has been submitted for an R&D100 award in 1995. In addition, it is high on the list of applications to be deployed across the entire U.S. by the NIIT (National Information Infrastructure Testbed, an industrial consortium working to develop the NII).

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